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Numerical simulation for the 3D seepage flow with fractional derivatives in porous media

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In this paper, the numerical simulation of the 3D seepage flow with fractional derivatives in porous media is considered under two special cases: non-continued seepage flow in uniform media (NCSF-UM) and continued seepage flow in non-uniform media (CSF-NUM). A fractional alternating direction implicit scheme (FADIS) for the NCSF-UM and a modified Douglas scheme (MDS) for the CSF-NUM are proposed. The stability, consistency and convergence of both FADIS and MDS in a bounded domain are discussed. A method for improving the speed of convergence by Richardson extrapolation for the MDS is also presented. Finally, numerical results are presented to support our theoretical analysis.

Keywords: seepage flow; fractional derivative; fractional alternating direction implicit scheme; modified Douglas scheme; stability and convergence; Richardson extrapolation.

1. Introduction

Seepage flow problems are discussed in many research fields, such as seepage hydraulics, groundwater hydraulics, groundwater dynamics and fluid dynamics in porous media (see Huang *et al.*, 1996; Thusyanthan & Madabhushi, 2003; Petford & Koenders, 2003; Chou *et al.*, 2006). Darcy (1856) derived the following result, the famous Darcy's law, through experiments of saturated flow of water through a column of soil:

$$q_x = K_x \frac{\partial P}{\partial x}, \quad q_y = K_y \frac{\partial P}{\partial y}, \quad q_z = K_z \frac{\partial P}{\partial z},$$

where P is the pressure; q_x , q_y and q_z are the velocity components in the x , y , z directions, respectively, and K_x , K_y and K_z are the percolation coefficients along the x , y , z directions, respectively.

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For heterogeneous media, under the assumptions of seepage flow continuity and Darcy's law, and by taking the main directions of the percolation coefficients as the coordinate directions exclusive of gravity, the partial differential equation (PDE) for single-phase isothermal seepage flow can be written as follows (see Rushton & Redshaw, 1979; Huang *et al.*, 1996; He, 1998; Mao *et al.*, 1999; Luo *et al.*, 2008):

$$\frac{1}{v} \frac{\partial P}{\partial t} = \frac{\partial}{\partial x} \left(K_x \frac{\partial P}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial P}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial P}{\partial z} \right) + f, \quad (x, y, z) \in \Omega, \quad (1.1)$$

with boundary condition

$$P(x, y, z, t)|_{\Gamma} = \Phi \quad (1.2)$$

and initial condition

$$P(x, y, z, 0) = \varphi(x, y, z), \quad (1.3)$$

where t is the time, $\frac{1}{v}$ is the specific storage coefficient, which is assumed constant, $f = f(x, y, z, t)$ is the source and sink term, Ω denotes the percolation domain and Γ is the boundary of Ω .

Equation (1.1) was discussed in some references, such as Equation (1–81) in Mao (2003), Equation (1–16) in Liggett & Liu (1983) and Equation (6.4.12) in Bear (1972), which was the 3D continuous equation for the pressure in homogeneous aquifer.

It should be noted that the above percolation equation (1.1) has been deduced under the assumptions of continuity of seepage flow and Darcy's law, which generally speaking is not valid for real seepage flow. He (1998) proposed the following modified Darcy's law, or generalized Darcy's law, with fractional Riemann–Liouville derivatives:

$$q_x = K_x \frac{\partial^{\alpha_1} P}{\partial x^{\alpha_1}}, \quad q_y = K_y \frac{\partial^{\alpha_2} P}{\partial y^{\alpha_2}}, \quad q_z = K_z \frac{\partial^{\alpha_3} P}{\partial z^{\alpha_3}}, \quad 0 < \alpha_1, \alpha_2, \alpha_3 < 1.$$

The fractional Riemann–Liouville derivative of order α is defined in Podlubny (1999) as

$$\frac{d^\alpha \psi(x)}{dx^\alpha} = \frac{1}{\Gamma(n - \alpha)} \frac{d^n}{dx^n} \int_0^x \frac{\psi(\xi)}{(x - \xi)^{1+\alpha-n}} d\xi, \quad (1.4)$$

where n is an integer such that $n - 1 < \alpha \leq n$.

A more general equation for seepage flow with fractional Riemann–Liouville derivatives was proposed by He (1998):

$$\begin{aligned} \frac{1}{v} \frac{\partial P(x, y, z, t)}{\partial t} = & \frac{\partial^{\beta_1}}{\partial x^{\beta_1}} \left(K_x \frac{\partial^{\alpha_1} P(x, y, z, t)}{\partial x^{\alpha_1}} \right) + \frac{\partial^{\beta_2}}{\partial y^{\beta_2}} \left(K_y \frac{\partial^{\alpha_2} P(x, y, z, t)}{\partial y^{\alpha_2}} \right) \\ & + \frac{\partial^{\beta_3}}{\partial z^{\beta_3}} \left(K_z \frac{\partial^{\alpha_3} P(x, y, z, t)}{\partial z^{\alpha_3}} \right) + f(x, y, z, t), \quad (x, y, z) \in \Omega, \end{aligned} \quad (1.5)$$

where $0 < \beta_1, \beta_2, \beta_3, \alpha_1, \alpha_2, \alpha_3 \leq 1$ and $1 < \beta_1 + \alpha_1, \beta_2 + \alpha_2, \beta_3 + \alpha_3 \leq 2$.

Fractional differential equations (FDEs) have been used in particular in groundwater hydrology to model the transport of passive tracers carried by fluid flow in a porous medium. However, the analytic solutions of most FDEs are not usually given explicitly. So many authors discussed the numerical solutions of the FDEs (see Liu *et al.*, 2004a,b; Meerschaert & Tadjeran, 2004; Shen & Liu, 2005;

Meerschaert *et al.*, 2006; Jafari & Daftardar-Gejji, 2006; Roop, 2006; Zhuang & Liu, 2006; Chen *et al.*, 2007, 2008; Lin & Liu, 2007; Liu *et al.*, 2007a,b; Shen *et al.*, 2008; Yu *et al.*, 2008; Zhang *et al.*, 2007; Zhuang *et al.*, 2008). However, published papers on the numerical methods of the higher-dimensional FDEs are sparse. This motivates us to consider effective numerical methods for the high-dimensional FDEs.

In this paper, we investigate the numerical solutions of the two special seepage flow cases: non-continued seepage flow in uniform media (NCSF-UM) and continued seepage flow in non-uniform media (CSF-NUM).

For convenience, we simplify the fractional seepage flow equation (1.5) to the following form:

$$\frac{\partial P}{\partial t} = \frac{\partial^{\beta_1}}{\partial x^{\beta_1}} \left(K_x \frac{\partial^{\alpha_1} P}{\partial x^{\alpha_1}} \right) + \frac{\partial^{\beta_2}}{\partial y^{\beta_2}} \left(K_y \frac{\partial^{\alpha_2} P}{\partial y^{\alpha_2}} \right) + \frac{\partial^{\beta_3}}{\partial z^{\beta_3}} \left(K_z \frac{\partial^{\alpha_3} P}{\partial z^{\alpha_3}} \right) + f(x, y, z), \quad (x, y, z) \in \Omega, \quad (1.6)$$

where Ω is the finite cuboid domain $[0, L_x] \times [0, L_y] \times [0, L_z]$ and the time range $t \in [0, T]$. We assume that the three percolation coefficients $K_x, K_y, K_z > 0$. We also assume that this fractional seepage flow equation has a unique and sufficiently smooth solution under the following boundary conditions:

$$\begin{aligned} P(0, y, z, t) = \Phi_1(y, z, t) = 0, \quad P(L_x, y, z, t) = \Phi_2(y, z, t), \\ P(x, 0, z, t) = \Phi_3(x, z, t) = 0, \quad P(x, L_y, z, t) = \Phi_4(x, z, t), \\ P(x, y, 0, t) = \Phi_5(x, y, t) = 0, \quad P(x, y, L_z, t) = \Phi_6(x, y, t), \end{aligned} \quad (1.7)$$

and initial condition

$$P(x, y, z, 0) = \varphi(x, y, z).$$

The operators $\frac{\partial^{\beta_1}}{\partial x^{\beta_1}}, \frac{\partial^{\alpha_1}}{\partial x^{\alpha_1}}, \frac{\partial^{\beta_2}}{\partial y^{\beta_2}}, \frac{\partial^{\alpha_2}}{\partial y^{\alpha_2}}, \frac{\partial^{\beta_3}}{\partial z^{\beta_3}}, \frac{\partial^{\alpha_3}}{\partial z^{\alpha_3}}$ in (1.6) are the fractional Riemann–Liouville derivatives of order $\beta_1, \alpha_1, \beta_2, \alpha_2, \beta_3, \alpha_3$ with respect to x, y, z , respectively.

Furthermore, when a function has a continuous $(n-1)$ th-order derivative and its n th-order derivative is integrable, its fractional derivatives in both Riemann–Liouville and Grünwald–Letnikov senses are coincident. The Grünwald–Letnikov fractional derivative is defined in Podlubny (1999) as follows:

$$\frac{d^\alpha \psi(x)}{dx^\alpha} = \frac{1}{\Gamma(-\alpha)} \lim_{h \rightarrow 0} \frac{1}{h^\alpha} \sum_{i=0}^{\lfloor \frac{x}{h} \rfloor} \frac{\Gamma(i-\alpha)}{\Gamma(i+1)} \psi(x-ih) \quad (1.8)$$

and the shifted Grünwald–Letnikov estimate is defined by Podlubny (1999) as

$$\frac{d^\alpha \psi(x)}{dx^\alpha} = \frac{1}{\Gamma(-\alpha)} \lim_{h \rightarrow 0} \frac{1}{h^\alpha} \sum_{i=0}^{\lfloor \frac{x}{h} \rfloor + 1} \frac{\Gamma(i-\alpha)}{\Gamma(i+1)} \psi(x-(i-1)h), \quad (1.9)$$

where $[x]$ means the integer part of x , h is the step and $\Gamma(\cdot)$ is the Gamma function. We denote the ‘normalized’ Grünwald weights by

$$g_{\alpha,i} = \frac{\Gamma(i-\alpha)}{\Gamma(-\alpha)\Gamma(i+1)} = (-1)^i \binom{\alpha}{i},$$

with the properties

$$g_{\alpha,i} \begin{cases} = 1, & i = 0, \\ < 0, & i = 1, 2, \dots, \end{cases} \quad g_{1+\alpha,i} \begin{cases} = 1, & i = 0, \\ < 0, & i = 1, \\ > 0, & i = 2, 3, \dots, \end{cases} \quad (1.10)$$

when $0 < \alpha < 1$. The $g_{\alpha,i}$ also satisfy the following properties:

$$\sum_{i=0}^{\infty} g_{\alpha,i} = (1-1)^{\alpha} = 0, \quad \sum_{i=0}^{\infty} g_{1+\alpha,i} = (1-1)^{1+\alpha} = 0. \quad (1.11)$$

The structure of the paper is as follows. In Section 2, a fractional alternating direction implicit scheme (FADIS) for NCSF-UM is proposed. The stability, consistency and convergence of the FADIS are then discussed. In Section 3, a modified Douglas scheme (MDS) for the CSF-UM is introduced, and the stability, consistency and convergence of the MDS are also investigated. A method for improving the speed of convergence by Richardson extrapolation is also presented. Finally, numerical results for both NCSF-UM and CSF-UM are given.

2. A non-continued seepage flow in uniform media

In this section, we consider the NCSF-UM, while the percolation coefficients K_x , K_y , K_z in (1.6) are constants. With the boundary conditions (1.7) and the composite property of two Grünwald–Letnikov fractional derivatives' composition (see Podlubny, 1999), NCSF-UM is given as

$$\begin{aligned} \frac{\partial P}{\partial t} &= K_x \frac{\partial^{\beta_1+\alpha_1} P}{\partial x^{\beta_1+\alpha_1}} + K_y \frac{\partial^{\beta_2+\alpha_2} P}{\partial y^{\beta_2+\alpha_2}} + K_z \frac{\partial^{\beta_3+\alpha_3} P}{\partial z^{\beta_3+\alpha_3}} + f \\ &:= K_x \frac{\partial^{\gamma_1} P}{\partial x^{\gamma_1}} + K_y \frac{\partial^{\gamma_2} P}{\partial y^{\gamma_2}} + K_z \frac{\partial^{\gamma_3} P}{\partial z^{\gamma_3}} + f, \quad (x, y, z) \in \Omega, \end{aligned} \quad (2.1)$$

where $\gamma_i = \beta_i + \alpha_i$.

Firstly, we construct an FADIS to solve the NCSF-UM. Next, we discuss the stability and convergence of the FADIS.

2.1 FADIS for NCSF-UM in a bounded cuboid domain

In order to derive the FADIS, we first discretize the space and time variables using

$$\begin{aligned} x_i &= ih_x, \quad i = 0, 1, 2, \dots, M_x, \quad h_x = \frac{L_x}{M_x}, \\ y_j &= jh_y, \quad j = 0, 1, 2, \dots, M_y, \quad h_y = \frac{L_y}{M_y}, \\ z_k &= kh_z, \quad k = 0, 1, 2, \dots, M_z, \quad h_z = \frac{L_z}{M_z}, \end{aligned}$$

and

$$t_n = n\tau, \quad n = 0, 1, 2, \dots, N, \quad \tau = \frac{T}{N},$$

where M_x, M_y, M_z, N are positive integers, h_x, h_y, h_z are the space (x -direction, y -direction and z -direction) and τ time steps.

The dependent variable P is then discretized by defining $P_{i,j,k}^n$ as the numerical approximation to $P(x_i, y_j, z_k, t_n)$. Similar notation gives $f_{i,j,k}^n = f(x_i, y_j, z_k, t_n)$. The initial condition is set as $P_{i,j,k}^0 = \varphi_{i,j,k} = \varphi(x_i, y_j, z_k)$, and the boundary conditions are set such that on the six sides of the domain $P_{0,j,k}^n = \Phi_1(y_j, z_k, t_n) = 0$, $P_{M_x,j,k}^n = \Phi_2(y_j, z_k, t_n)$, $P_{i,0,k}^n = \Phi_3(x_i, z_k, t_n) = 0$, $P_{i,M_y,k}^n = \Phi_4(x_i, z_k, t_n)$, $P_{i,j,0}^n = \Phi_5(x_i, y_j, t_n) = 0$ and $P_{i,j,M_z}^n = \Phi_6(x_i, y_j, t_n)$.

To discretize the NCSF-UM, we approximate the first-order derivative $\frac{\partial P}{\partial t}$ in NCSF-UM using the first-order difference quotient. Furthermore, we assume that it has first-order continuous derivative and its second-order derivative is integrable, with respect to the space variables, so that we can discretize the operator $\frac{\partial^{\gamma_1}}{\partial x^{\gamma_1}}, \frac{\partial^{\gamma_2}}{\partial y^{\gamma_2}}, \frac{\partial^{\gamma_3}}{\partial z^{\gamma_3}}$ in NCSF-UM using the shifted definition of the Grünwald–Letnikov fractional derivative (1.9).

Discretizing all variables, we obtain the following simple implicit finite-difference scheme for NCSF-UM:

$$\begin{aligned} \frac{P_{i,j,k}^{n+1} - P_{i,j,k}^n}{\tau} &= \frac{K_x}{h_x^{\gamma_1}} \sum_{s=0}^{i+1} g_{\gamma_1,s} P_{i+1-s,j,k}^{n+1} + \frac{K_y}{h_y^{\gamma_2}} \sum_{s=0}^{j+1} g_{\gamma_2,s} P_{i,j+1-s,k}^{n+1} \\ &+ \frac{K_z}{h_z^{\gamma_3}} \sum_{s=0}^{k+1} g_{\gamma_3,s} P_{i,j,k+1-s}^{n+1} + f_{i,j,k}^{n+1}. \end{aligned} \quad (2.2)$$

We consider the following fractional partial differential discrete operator:

$$\delta_x^{\gamma_1} P_{i,j,k}^{n+1} = \frac{1}{h_x^{\gamma_1}} \sum_{s=0}^{i+1} g_{\gamma_1,s} P_{i+1-s,j,k}^{n+1}, \quad (2.3)$$

which is an $O(h_x)$ approximation to the γ_1 -order Grünwald–Letnikov shifted fractional derivative (1.9) (see Meerschaert & Tadjeran, 2004). Similarly, the following fractional partial differential discrete operators,

$$\delta_y^{\gamma_2} P_{i,j,k}^{n+1} = \frac{1}{h_y^{\gamma_2}} \sum_{s=0}^{j+1} g_{\gamma_2,s} P_{i,j+1-s,k}^{n+1}, \quad \delta_z^{\gamma_3} P_{i,j,k}^{n+1} = \frac{1}{h_z^{\gamma_3}} \sum_{s=0}^{k+1} g_{\gamma_3,s} P_{i,j,k+1-s}^{n+1}, \quad (2.4)$$

are $O(h_y)$ and $O(h_z)$ approximations of the γ_2 - and γ_3 -order Grünwald–Letnikov shifted fractional derivatives (1.9), respectively.

With these definitions, the implicit difference scheme (2.2) may be written in the following form:

$$(I - K_x \tau \delta_x^{\gamma_1} - K_y \tau \delta_y^{\gamma_2} - K_z \tau \delta_z^{\gamma_3}) P_{i,j,k}^{n+1} = P_{i,j,k}^n + \tau f_{i,j,k}^{n+1}. \quad (2.5)$$

The implicit difference scheme (2.2) for NCSF-UM has a local truncation error of the form $O(\tau) + O(h_x) + O(h_y) + O(h_z)$ and is unconditionally stable (refer to the proof of Theorem 2.1 in this paper). Unfortunately, (2.2) provides us with a linear system of equations for calculating the difference solution $P_{i,j,k}^{n+1}$, that does not have the good property of the coefficient matrix being sparse and band structured as for the classical case. That is to say, at each time step, the implicit difference scheme (2.2) requires the solution of a very large dense linear system of equations with $(M_x - 1) \cdot (M_y - 1) \cdot (M_z - 1)$ unknowns,

which is computationally intensive to solve. It is therefore necessary to construct other numerical methods that are unconditionally stable, with less computational overheads for solution.

For this purpose, we adopt the alternating direction implicit method to design an implicit difference scheme for each direction. Our aim is to divide the calculation into three steps with reduced calculation. In the first step, we solve the problem in the x -direction, in the second step, we solve the problem in the y -direction, finally in the third step we solve the problem in the z -direction. For example, we introduce an additional higher-order term

$$(K_x K_y \tau^2 \delta_x^{y1} \delta_y^{y2} + K_x K_z \tau^2 \delta_x^{y1} \delta_z^{y3} + K_y K_z \tau^2 \delta_y^{y2} \delta_z^{y3} - K_x K_y K_z \tau^3 \delta_x^{y1} \delta_y^{y2} \delta_z^{y3}) P_{i,j,k}^{n+1} \quad (2.6)$$

to the left side of (2.5), enabling the following scheme to be constructed:

$$(I - K_x \tau \delta_x^{y1})(I - K_y \tau \delta_y^{y2})(I - K_z \tau \delta_z^{y3}) P_{i,j,k}^{n+1} = P_{i,j,k}^n + \tau f_{i,j,k}^{n+1}. \quad (2.7)$$

Hence, we obtain the FADIS at time t_{n+1} :

$$(I - K_x \tau \delta_x^{y1}) P_{i,j,k}^{n+1/3} = P_{i,j,k}^n + \tau f_{i,j,k}^{n+1}, \quad (2.8)$$

$$(I - K_y \tau \delta_y^{y2}) P_{i,j,k}^{n+2/3} = P_{i,j,k}^{n+1/3} \quad (2.9)$$

and

$$(I - K_z \tau \delta_z^{y3}) P_{i,j,k}^{n+1} = P_{i,j,k}^{n+2/3}. \quad (2.10)$$

Thus, we require three steps to solve the NCSF-UM in one time step.

Step 1: We solve the problem in the x -direction (for each fixed (y_j, z_k)) to obtain the intermediate solution $P_{i,j,k}^{n+1/3}$ from (2.8).

Step 2: We solve the problem in the y -direction (for each (x_i, z_k)) to obtain the intermediate solution $P_{i,j,k}^{n+2/3}$ from (2.9) using information compiled during Step 1.

Step 3: We solve in the z -direction (for each (x_i, y_j)) from (2.10) using information compiled during Step 2.

Together with the boundary values $P_{0,j,k}^{n+1/3}$ and $P_{M_x,j,k}^{n+1/3}$ calculated below, the coefficient matrix $A = (a_{s,t})$ of the linear system (2.8) can be obtained: for each fixed (j, k) ,

$$a_{s,t} = \begin{cases} 0, & t \geq s + 2, s = 1, 2, \dots, M_x - 3, \\ -\frac{K_x \tau}{h_x^{y1}} g_{\gamma 1,0}, & t = s + 1, s = 1, 2, \dots, M_x - 2, \\ 1 - \frac{K_x \tau}{h_x^{y1}} g_{\gamma 1,1}, & t = s = 1, 2, \dots, M_x - 1, \\ -\frac{K_x \tau}{h_x^{y1}} g_{\gamma 1,s-t+1}, & t \leq s - 1, s = 2, 3, \dots, M_x - 1. \end{cases} \quad (2.11)$$

Furthermore with the boundary values $P_{i,0,k}^{n+2/3}$ and $P_{i,M_y,k}^{n+2/3}$ calculated below, the coefficient matrix $B = (b_{s,t})$ of the linear system (2.9) can be obtained, and for each fixed (i, k) its form is similar to the matrix A in (2.11).

Finally, with the given boundary conditions $P_{i,j,0}^{n+1}$ and P_{i,j,M_z}^{n+1} , the coefficient matrix $C = (c_{s,t})$ of the linear system (2.10) can be obtained, and for each fixed (i, j) its form is similar to the matrix A in (2.11).

Similar to the alternating direction method for the classical integer-order PDE, to maintain the approximation order, it is necessary to provide the additional boundary values in the x -direction $P_{0,j,k}^{n+1/3}$, $P_{M_x,j,k}^{n+1/3}$ and in the y -direction $P_{i,0,k}^{n+2/3}$, $P_{i,M_y,k}^{n+2/3}$, when solving the system of equations with coefficient matrices A and B . For example, we provide the additional boundary values $P_{0,j,k}^{n+1/3}$, $P_{M_x,j,k}^{n+1/3}$, which can be obtained as

$$P_{i,j,k}^{n+1/3} = (I - K_y \tau \delta_y^{\gamma_2})(I - K_z \tau \delta_z^{\gamma_3})P_{i,j,k}^{n+1}, \quad i = 0, M_x,$$

where $j = 1, 2, \dots, M_y - 1$, $k = 1, 2, \dots, M_z - 1$, $n = 0, 1, \dots, N - 1$, and $P_{i,0,k}^{n+2/3}$, $P_{i,M_y,k}^{n+2/3}$ can be obtained from

$$P_{i,j,k}^{n+2/3} = (I - K_z \tau \delta_z^{\gamma_3})P_{i,j,k}^{n+1}, \quad j = 0, M_y,$$

where $i = 1, 2, \dots, M_x - 1$, $k = 1, 2, \dots, M_z - 1$, $n = 0, 1, \dots, N - 1$.

From the three coefficient matrices, it can be seen that at each time step, it is just required to solve, for each fixed (j, k) (every layer in the x -direction) or each fixed (i, k) (every layer in the y -direction) or each fixed (i, j) (every layer in the z -direction), the solution of a linear system of equations with a upper triangular coefficient matrix and $M_x - 1$ or $M_y - 1$ or $M_z - 1$ unknowns.

2.2 Analysis of stability and consistency of the FADIS

In this section, we first demonstrate that the FADIS is unconditionally stable for the NCSF-UM (2.1) using the Fourier method (see Ciarlet & Lions, 1990).

The numerical solution is governed by the difference equations (2.8–2.10). Eliminating the medial variables $P_{i,j,k}^{n+1/3}$, $P_{i,j,k}^{n+2/3}$ leads to (2.7).

To investigate the stability of FADIS, we assume that the initial error $\varepsilon_{i,j,k}^0$ is introduced only when the initial condition is discretized. We also assume that the set of inner grid points is denoted as $\Omega' = \{(i, j, k) | i = 1, 2, \dots, M_x - 1, j = 1, 2, \dots, M_y - 1, k = 1, 2, \dots, M_z - 1\}$, $\partial\Omega$ the set of boundary points by $i = 0, M_x$; $j = 0, M_y$ or $k = 0, M_z$. Thus, the error $\varepsilon_{i,j,k}^n$, which is accumulated from the initial error $\varepsilon_{i,j,k}^0$ in the course of solving the difference equations (2.8–2.10), satisfies

$$\begin{cases} (I - K_x \tau \delta_x^{\gamma_1})(I - K_y \tau \delta_y^{\gamma_2})(I - K_z \tau \delta_z^{\gamma_3})\varepsilon_{i,j,k}^{n+1} = \varepsilon_{i,j,k}^n, & i, j, k \in \Omega', 0 \leq n < N, \\ \varepsilon_{i,j,k}^0 \text{ is given,} & i, j, k \in \Omega', \\ \varepsilon_{0,j,k}^n = \varepsilon_{M_x,j,k}^n = \varepsilon_{i,0,k}^n = \varepsilon_{i,M_y,k}^n = \varepsilon_{i,j,0}^n = \varepsilon_{i,j,M_z}^n = 0, & 0 \leq n \leq N. \end{cases}$$

If we set $\varepsilon_{i,j,k}^n = \zeta_n e^{\tilde{i}(\tilde{q}_x i h_x + \tilde{q}_y j h_y + \tilde{q}_z k h_z)}$, where $\tilde{q}_x, \tilde{q}_y, \tilde{q}_z$ are three real spatial wave numbers, \tilde{i} is the imaginary unit, considering the definition of $\delta_x^{\gamma_1}$, $\delta_y^{\gamma_2}$, $\delta_z^{\gamma_3}$, then

$$\begin{aligned} & \zeta_{n+1} \left[e^{\tilde{i}\tilde{q}_x i h_x} - \frac{K_x \tau}{h_x^{\gamma_1}} \sum_{s=0}^{i+1} g_{\gamma_1,s} e^{\tilde{i}\tilde{q}_x (i+1-s)h_x} \right] \\ & \left[e^{\tilde{i}\tilde{q}_y j h_y} - \frac{K_y \tau}{h_y^{\gamma_2}} \sum_{s=0}^{j+1} g_{\gamma_2,s} e^{\tilde{i}\tilde{q}_y (j+1-s)h_y} \right] \end{aligned}$$

$$\begin{aligned}
& \left[e^{\tilde{q}_z k h_z} - \frac{K_z \tau}{h_z^{\gamma_3}} \sum_{s=0}^{k+1} g_{\gamma_3, s} e^{\tilde{q}_z (k+1-s) h_z} \right] \\
&= \zeta_n e^{\tilde{q}_x i h_x} e^{\tilde{q}_y j h_y} e^{\tilde{q}_z k h_z}.
\end{aligned} \tag{2.12}$$

The numerical method is stable if $|\zeta_{k+1}| \leq |\zeta_k|$. Dividing (2.12) by $e^{\tilde{q}_x i h_x + \tilde{q}_y j h_y + \tilde{q}_z k h_z}$, denoting the left and right sides as LS and RS, respectively, and then taking the complex modulus, we obtain

$$\begin{aligned}
|\text{LS}| &= |\zeta_{n+1}| \left| 1 - \frac{K_x \tau}{h_x^{\gamma_1}} \sum_{s=0}^{i+1} g_{\gamma_1, s} e^{-\tilde{q}_x (s-1) h_x} \right| \\
&\quad \times \left| 1 - \frac{K_y \tau}{h_y^{\gamma_2}} \sum_{s=0}^{j+1} g_{\gamma_2, s} e^{-\tilde{q}_y (s-1) h_y} \right| \left| 1 - \frac{K_z \tau}{h_z^{\gamma_3}} \sum_{s=0}^{k+1} g_{\gamma_3, s} e^{-\tilde{q}_z (s-1) h_z} \right| \\
&= |\zeta_{n+1}| \left| 1 - \frac{K_x \tau}{h_x^{\gamma_1}} g_{\gamma_1, 1} - \frac{K_x \tau}{h_x^{\gamma_1}} \sum_{s=0, \neq 1}^{i+1} g_{\gamma_1, s} e^{-\tilde{q}_x (s-1) h_x} \right| \\
&\quad \times \left| 1 - \frac{K_y \tau}{h_y^{\gamma_2}} g_{\gamma_2, 1} - \frac{K_y \tau}{h_y^{\gamma_2}} \sum_{s=0, \neq 1}^{j+1} g_{\gamma_2, s} e^{-\tilde{q}_y (s-1) h_y} \right| \\
&\quad \times \left| 1 - \frac{K_z \tau}{h_z^{\gamma_3}} g_{\gamma_3, 1} - \frac{K_z \tau}{h_z^{\gamma_3}} \sum_{s=0, \neq 1}^{k+1} g_{\gamma_3, s} e^{-\tilde{q}_z (s-1) h_z} \right|.
\end{aligned}$$

Utilizing repetitively the complex triangular inequality

$$|z_1 - z_2| \geq ||z_1| - |z_2||$$

and the property

$$|e^{i\theta}| = 1,$$

we have

$$\begin{aligned}
|\text{LS}| &\geq |\zeta_{n+1}| \left| 1 - \frac{K_x \tau}{h_x^{\gamma_1}} g_{\gamma_1, 1} \right| - \left| \frac{K_x \tau}{h_x^{\gamma_1}} g_{\gamma_1, 0} \right| - \left| \frac{K_x \tau}{h_x^{\gamma_1}} g_{\gamma_1, 2} \right| - \cdots - \left| \frac{K_x \tau}{h_x^{\gamma_1}} g_{\gamma_1, i+1} \right| \\
&\quad \times \left| 1 - \frac{K_y \tau}{h_y^{\gamma_2}} g_{\gamma_2, 1} \right| - \left| \frac{K_y \tau}{h_y^{\gamma_2}} g_{\gamma_2, 0} \right| - \left| \frac{K_y \tau}{h_y^{\gamma_2}} g_{\gamma_2, 2} \right| - \cdots - \left| \frac{K_y \tau}{h_y^{\gamma_2}} g_{\gamma_2, j+1} \right| \\
&\quad \times \left| 1 - \frac{K_z \tau}{h_z^{\gamma_3}} g_{\gamma_3, 1} \right| - \left| \frac{K_z \tau}{h_z^{\gamma_3}} g_{\gamma_3, 0} \right| - \left| \frac{K_z \tau}{h_z^{\gamma_3}} g_{\gamma_3, 2} \right| - \cdots - \left| \frac{K_z \tau}{h_z^{\gamma_3}} g_{\gamma_3, k+1} \right|.
\end{aligned}$$

Due to the properties of $g_{\gamma,i}$ given in (1.10), we have that for $1 < \gamma < 2$, $g_{\gamma,1} < 0$ and $g_{\gamma,i} > 0$ for $i \neq 1$, noting that $K_x > 0$, $K_y > 0$ and $K_z > 0$. Thus,

$$\begin{aligned} |\text{LS}| &\geq |\zeta_{n+1}| \left| 1 - \frac{K_x \tau}{h_x^{\gamma_1}} g_{\gamma_1,1} - \frac{K_x \tau}{h_x^{\gamma_1}} g_{\gamma_1,0} - \frac{K_x \tau}{h_x^{\gamma_1}} g_{\gamma_1,2} - \cdots - \frac{K_x \tau}{h_x^{\gamma_1}} g_{\gamma_1,i+1} \right| \\ &\quad \times \left| 1 - \frac{K_y \tau}{h_y^{\gamma_2}} g_{\gamma_2,1} - \frac{K_y \tau}{h_y^{\gamma_2}} g_{\gamma_2,0} - \frac{K_y \tau}{h_y^{\gamma_2}} g_{\gamma_2,2} - \cdots - \frac{K_y \tau}{h_y^{\gamma_2}} g_{\gamma_2,j+1} \right| \\ &\quad \times \left| 1 - \frac{K_z \tau}{h_z^{\gamma_3}} g_{\gamma_3,1} - \frac{K_z \tau}{h_z^{\gamma_3}} g_{\gamma_3,0} - \frac{K_z \tau}{h_z^{\gamma_3}} g_{\gamma_3,2} - \cdots - \frac{K_z \tau}{h_z^{\gamma_3}} g_{\gamma_3,k+1} \right| \\ &= |\zeta_{n+1}| \left| 1 - \frac{K_x \tau}{h_x^{\gamma_1}} \sum_{s=0}^{i+1} g_{\gamma_1,s} \right| \left| 1 - \frac{K_y \tau}{h_y^{\gamma_2}} \sum_{s=0}^{j+1} g_{\gamma_2,s} \right| \left| 1 - \frac{K_z \tau}{h_z^{\gamma_3}} \sum_{s=0}^{k+1} g_{\gamma_3,s} \right|. \end{aligned}$$

From (1.11), it follows that

$$\sum_{s=0}^l g_{\gamma,s} < \sum_{s=0}^{\infty} g_{\gamma,s} = 0, \quad \text{for } l, 1 < \gamma < 2,$$

and with the conditions $K_x > 0$, $K_y > 0$ and $K_z > 0$. Then

$$|\text{LS}| \geq |\zeta_{n+1}|.$$

From (2.12), we have

$$|\text{RS}| = |\zeta_n|.$$

Therefore, we have

$$|\zeta_{n+1}| \leq |\zeta_n|, \quad (2.13)$$

so the following theorem is obtained.

THEOREM 2.1 The FADIS, defined by (2.7), is unconditionally stable for $1 < \gamma_1, \gamma_2, \gamma_3 < 2$.

In a similar manner outlined above to obtain (2.13), the one-step method (2.8), (2.9) or (2.10) of the FADIS can also be shown to be unconditionally stable.

To obtain the consistency of the FADIS, note that the time difference operator in (2.5) has a local truncation error of order $O(\tau)$, and the three space difference operators in (2.5) have local truncation errors of orders $O(h_x)$, $O(h_y)$ and $O(h_z)$, respectively, which was proved in Meerschaert & Tadjeran (2004). The only remaining term in the local error of the FADIS is the additional higher-order term (2.6).

From Lemma 2.1 (see Meerschaert *et al.*, 2006) below we can show that the additional term (2.6) is indeed of higher order, i.e. $O(\tau^2)$.

LEMMA 2.1 Let $r > \alpha + \beta + 3$ be an integer. Then for $f \in W^{r,1}(R^2)$,

$$\frac{\partial^\beta}{\partial y^\beta} \frac{\partial^\alpha}{\partial x^\alpha} f(x, y) = \frac{1}{h_x^\alpha} \frac{1}{h_y^\beta} \sum_{s=0}^{\infty} \sum_{t=0}^{\infty} g_{\alpha,s} g_{\beta,t} f(x - (s-m)h_x, y - (t-n)h_y) + O(h_x + h_y) \quad (2.14)$$

uniformly in $(x, y) \in R^2$, where m, n are positive integers.

In our paper, we utilize the constants $m, n = 1$, and from (2.14) we have the results

$$\frac{\partial^{\gamma_1}}{\partial x^{\gamma_1}} \frac{\partial^{\gamma_2}}{\partial y^{\gamma_2}} f(x, y, z) = \delta_x^{\gamma_1} \delta_y^{\gamma_2} f(x, y, z) + O(h_x + h_y),$$

$$\frac{\partial^{\gamma_1}}{\partial x^{\gamma_1}} \frac{\partial^{\gamma_3}}{\partial z^{\gamma_3}} f(x, y, z) = \delta_x^{\gamma_1} \delta_z^{\gamma_3} f(x, y, z) + O(h_x + h_z),$$

$$\frac{\partial^{\gamma_2}}{\partial y^{\gamma_2}} \frac{\partial^{\gamma_3}}{\partial z^{\gamma_3}} f(x, y, z) = \delta_y^{\gamma_2} \delta_z^{\gamma_3} f(x, y, z) + O(h_y + h_z).$$

Similar to Lemma 2.1, the following approximation is obtained:

$$\frac{\partial^{\gamma_1}}{\partial x^{\gamma_1}} \frac{\partial^{\gamma_2}}{\partial y^{\gamma_2}} \frac{\partial^{\gamma_3}}{\partial z^{\gamma_3}} f(x, y, z) = \delta_x^{\gamma_1} \delta_y^{\gamma_2} \delta_z^{\gamma_3} f(x, y, z) + O(h_x + h_y + h_z),$$

which leads to the following theorem.

THEOREM 2.2 The FADIS (2.7) is consistent to the NCSF-UM (2.1) with order $O(\tau) + O(h_x + h_y + h_z)$.

We show above that the FADIS is consistent and stable, then by Lax's equivalence theorem (see Smith, 1990), it converges at the rate $O(\tau) + O(h_x) + O(h_y) + O(h_z)$.

We show in Section 3 that it is possible to obtain a more higher-order approximation for (2.1).

3. A continued seepage flow in non-uniform media

In this section, we consider the problem of CSF-NUM, i.e. $\beta_1 = \beta_2 = \beta_3 = 1$, $K_x = K_x(x, y, z)$, $K_y = K_y(x, y, z)$ and $K_z = K_z(x, y, z)$ in (1.5):

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial x} \left(K_x \frac{\partial^{\alpha_1} P}{\partial x^{\alpha_1}} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial^{\alpha_2} P}{\partial y^{\alpha_2}} \right) + \frac{\partial P}{\partial z} \left(K_z \frac{\partial^{\alpha_3} P}{\partial z^{\alpha_3}} \right) + f,$$

with the initial and boundary conditions and the property of the composition of the integer-order and fractional-order derivatives (see Podlubny, 1999), which can be rewritten as the following equivalent 3D space fractional advection–diffusion equation:

$$\left\{ \begin{array}{l} \frac{\partial P}{\partial t} = K'_x \frac{\partial^{\alpha_1} P}{\partial x^{\alpha_1}} + K_x \frac{\partial^{1+\alpha_1} P}{\partial x^{1+\alpha_1}} + K'_y \frac{\partial^{\alpha_2} P}{\partial y^{\alpha_2}} + K_y \frac{\partial^{1+\alpha_2} P}{\partial y^{1+\alpha_2}} + K'_z \frac{\partial^{\alpha_3} P}{\partial z^{\alpha_3}} + K_z \frac{\partial^{1+\alpha_3} P}{\partial z^{1+\alpha_3}} + f, \\ P(x, y, z, 0) = \varphi(x, y, z), \\ P(0, y, z, t) = \phi_1(y, z, t) = 0, \quad P(L_x, y, z, t) = \phi_2(y, z, t), \\ P(x, 0, z, t) = \phi_3(x, z, t) = 0, \quad P(x, L_y, z, t) = \phi_4(x, z, t), \\ P(x, y, 0, t) = \phi_5(x, y, t) = 0, \quad P(x, y, L_z, t) = \phi_6(x, y, t), \end{array} \right. \quad (3.1)$$

on a finite cuboid domain $[0, L_x] \times [0, L_y] \times [0, L_z]$ with $0 < \alpha_1, \alpha_2, \alpha_3 \leq 1$, the time range $t \in [0, T]$ and $K'_x = \frac{\partial K_x(x, y, z)}{\partial x}$, $K'_y = \frac{\partial K_y(x, y, z)}{\partial y}$, $K'_z = \frac{\partial K_z(x, y, z)}{\partial z}$. We assume that the three advection coefficients $K'_x(x, y, z)$, $K'_y(x, y, z)$, $K'_z(x, y, z) \leq 0$ and the three dispersion coefficients $K_x(x, y, z)$,

$K_y(x, y, z)$, $K_z(x, y, z) > 0$ (Roop, 2004; Liu *et al.*, 2004b; Meerschaert & Tadjeran, 2004). Under these assumptions, this FDE has a unique and sufficiently smooth solution for the given initial and boundary conditions, which can be proved (see Roop, 2004).

In this section, we propose an MDS. This approach is based on an alternating direction implicit method combined with spatial extrapolation to obtain temporally and spatially more than first-order accurate numerical estimates. Then we consider the stability, consistency and convergence of the MDS.

3.1 An MDS for CSF-NUM in a bounded cuboid domain

In order to obtain the MDS, we first discretize the space and time variables at the grid points and time instants as given in the previous part.

The dependent variable P is discretized by defining $P_{i,j,k}^n$ as the numerical approximations to $P(x_i, y_j, z_k, t_n)$. Similar notation gives $K'_{x_{i,j,k}} = K'_x(x_i, y_j, z_k)$, $K_{x_{i,j,k}} = K_x(x_i, y_j, z_k)$, $K'_{y_{i,j,k}} = K'_y(x_i, y_j, z_k)$, $K_{y_{i,j,k}} = K_y(x_i, y_j, z_k)$, $K'_{z_{i,j,k}} = K'_z(x_i, y_j, z_k)$, $K_{z_{i,j,k}} = K_z(x_i, y_j, z_k)$ and $f_{i,j,k}^n = f(x_i, y_j, z_k, t_n)$. The initial condition is given by $P_{i,j,k}^0 = \phi_{i,j,k} = \phi(x_i, y_j, z_k)$, and the boundary conditions are given on the six sides of the domain by $P_{0,j,k}^n = \phi_1(y_j, z_k, t_n) = 0$, $P_{M_x,j,k}^n = \phi_2(y_j, z_k, t_n)$, $P_{i,0,k}^n = \phi_3(x_i, z_k, t_n) = 0$, $P_{i,M_y,k}^n = \phi_4(x_i, z_k, t_n)$, $P_{i,j,0}^n = \phi_5(x_i, y_j, t_n) = 0$ and $P_{i,j,M_z}^n = \phi_6(x_i, y_j, t_n)$.

Similar to the approximation derived in Section 2, we approximate the first-order derivative $\frac{\partial P}{\partial t}$ by the first-order difference quotient, the fractional derivatives $\frac{\partial^{\alpha_1} P}{\partial x^{\alpha_1}}$, $\frac{\partial^{\alpha_2} P}{\partial y^{\alpha_2}}$, $\frac{\partial^{\alpha_3} P}{\partial z^{\alpha_3}}$ by (1.8) and the fractional derivatives $\frac{\partial^{1+\alpha_1} P}{\partial x^{1+\alpha_1}}$, $\frac{\partial^{1+\alpha_2} P}{\partial y^{1+\alpha_2}}$, $\frac{\partial^{1+\alpha_3} P}{\partial z^{1+\alpha_3}}$ by (1.9), respectively. Then, we obtain a simple implicit finite-difference scheme for CSF-NUM, by which the linear system of equations again has a dense coefficient matrix. It is necessary to construct another numerical method that is unconditionally stable, with less computational overheads.

For this purpose, we adopt the alternating direction implicit method to design an implicit difference scheme—MDS. The classical Douglas scheme of the alternating direction method for the integer-order diffusion equation

$$\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} + \frac{\partial^2 P}{\partial z^2}$$

has the form (see Ciarlet & Lions, 1990)

$$\begin{cases} (I - \frac{r}{2}\delta_x^2) \left(\frac{P_{i,j,k}^{n+1/3} - P_{i,j,k}^n}{\tau} \right) = \frac{1}{h^2} (\delta_x^2 + \delta_y^2 + \delta_z^2) P_{i,j,k}^n, \\ \frac{P_{i,j,k}^{n+2/3} - P_{i,j,k}^{n+1/3}}{\tau/2} = \frac{1}{h^2} \delta_y^2 (P_{i,j,k}^{n+2/3} - P_{i,j,k}^n), \\ \frac{P_{i,j,k}^{n+1} - P_{i,j,k}^{n+2/3}}{\tau/2} = \frac{1}{h^2} \delta_z^2 (P_{i,j,k}^{n+1} - P_{i,j,k}^n), \end{cases}$$

where $r = \tau/h^2$ and δ_x^2 , δ_y^2 and δ_z^2 are the central difference quotient operators in the three directions.

We construct the MDS in one time step for (3.1) as follows:

$$\left\{ \begin{aligned} & \left[I - \frac{\tau}{2} (K'_x \tilde{\delta}_x^{\alpha_1} + K_x \delta_x^{1+\alpha_1}) \right] \left(\frac{P_{i,j,k}^{n+1/3} - P_{i,j,k}^n}{\tau} \right) \\ &= (K'_x \tilde{\delta}_x^{\alpha_1} + K_x \delta_x^{1+\alpha_1} + K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2} + K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3}) P_{i,j,k}^n \\ &+ \frac{\tau^2}{4} (K'_x \tilde{\delta}_x^{\alpha_1} + K_x \delta_x^{1+\alpha_1}) (K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2}) (K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3}) P_{i,j,k}^n + \frac{1}{2} (f_{i,j,k}^{n+1} + f_{i,j,k}^n), \\ & \frac{P_{i,j,k}^{n+2/3} - P_{i,j,k}^{n+1/3}}{\tau/2} = (K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3}) (P_{i,j,k}^{n+1/3} - P_{i,j,k}^n), \\ & \frac{P_{i,j,k}^{n+1} - P_{i,j,k}^{n+2/3}}{\tau/2} = (K'_x \tilde{\delta}_x^{\alpha_1} + K_x \delta_x^{1+\alpha_1}) (P_{i,j,k}^{n+2/3} - P_{i,j,k}^{n+1/3}), \end{aligned} \right.$$

with the definition of fractional partial differential operators given by

$$\begin{aligned} \tilde{\delta}_x^{\alpha_1} P_{i,j,k}^n &= \frac{1}{h_x^{\alpha_1}} \sum_{s=0}^i g_{\alpha_1,s} P_{i-s,j,k}^n, & \delta_x^{1+\alpha_1} P_{i,j,k}^n &= \frac{1}{h_x^{1+\alpha_1}} \sum_{s=0}^{i+1} g_{1+\alpha_1,s} P_{i+1-s,j,k}^n, \\ \tilde{\delta}_y^{\alpha_2} P_{i,j,k}^n &= \frac{1}{h_y^{\alpha_2}} \sum_{s=0}^j g_{\alpha_2,s} P_{i,j-s,k}^n, & \delta_y^{1+\alpha_2} P_{i,j,k}^n &= \frac{1}{h_y^{1+\alpha_2}} \sum_{s=0}^{j+1} g_{1+\alpha_2,s} P_{i,j+1-s,k}^n, \\ \tilde{\delta}_z^{\alpha_3} P_{i,j,k}^n &= \frac{1}{h_z^{\alpha_3}} \sum_{s=0}^k g_{\alpha_3,s} P_{i,j,k-s}^n, & \delta_z^{1+\alpha_3} P_{i,j,k}^n &= \frac{1}{h_z^{1+\alpha_3}} \sum_{s=0}^{k+1} g_{1+\alpha_3,s} P_{i,j,k+1-s}^n \end{aligned} \quad (3.2)$$

and the symbol $K'_x, K_x, K'_y, K_y, K'_z, K_z$ are short for $K'_{x_{i,j,k}}, K_{x_{i,j,k}}, K'_{y_{i,j,k}}, K_{y_{i,j,k}}, K'_{z_{i,j,k}}, K_{z_{i,j,k}}$, respectively.

When solving the problem (3.1) in the layer $t = t_{n+1}$, we write the MDS in the form

$$\begin{aligned} & \left[I - \frac{\tau}{2} (K'_x \tilde{\delta}_x^{\alpha_1} + K_x \delta_x^{1+\alpha_1}) \right] P_{i,j,k}^{n+1/3} \\ &= \left[I + \frac{\tau}{2} (K'_x \tilde{\delta}_x^{\alpha_1} + K_x \delta_x^{1+\alpha_1}) \right] P_{i,j,k}^n \\ &+ \frac{\tau^3}{4} (K'_x \tilde{\delta}_x^{\alpha_1} + K_x \delta_x^{1+\alpha_1}) (K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2}) (K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3}) P_{i,j,k}^n \\ &+ \tau (K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2} + K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3}) P_{i,j,k}^n + \frac{\tau}{2} (f_{i,j,k}^{n+1} + f_{i,j,k}^n), \end{aligned} \quad (3.3)$$

$$\left[I - \frac{\tau}{2} (K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2}) \right] P_{i,j,k}^{n+2/3} = P_{i,j,k}^{n+1/3} - \frac{\tau}{2} (K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2}) P_{i,j,k}^n, \quad (3.4)$$

$$\left[I - \frac{\tau}{2} (K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3}) \right] P_{i,j,k}^{n+1} = P_{i,j,k}^{n+2/3} - \frac{\tau}{2} (K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3}) P_{i,j,k}^n. \quad (3.5)$$

Thus, we require three steps to solve the numerical solution in one time step:

Step 1: We solve the problem in the x -direction (for each fixed (y_j, z_k)) to obtain the intermediate solution $P_{i,j,k}^{n+1/3}$ from (3.3).

Step 2: We solve in the y -direction (for each (x_i, z_k)) to obtain the intermediate solution $P_{i,j,k}^{n+2/3}$ from (3.4) using information compiled during Step 1.

Step 3: We solve in the z -direction (for each (x_i, y_j)) from (3.5) using information compiled during Step 2.

To maintain the approximation order when solving the systems of equations (3.3), (3.4) and (3.5), we provide the additional boundary values $P_{0,j,k}^{n+1/3}$, $P_{M_x,j,k}^{n+1/3}$ in the x -direction and $P_{i,0,k}^{n+2/3}$, $P_{i,M_y,k}^{n+2/3}$ in the y -direction according to the following method. From (3.5) we have the following boundary values after letting $j = 0$ and $j = M_y$:

$$\begin{cases} P_{i,0,k}^{n+2/3} = P_{i,0,k}^{n+1} - \frac{\tau}{2}(K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3})(P_{i,0,k}^{n+1} - P_{i,0,k}^n), \\ P_{i,M_y,k}^{n+2/3} = P_{i,M_y,k}^{n+1} - \frac{\tau}{2}(K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3})(P_{i,M_y,k}^{n+1} - P_{i,M_y,k}^n), \end{cases} \quad (3.6)$$

where $P_{i,0,k}^n = \Phi_3(x_i, z_k, t_n)$, $P_{i,M_y,k}^n = \Phi_4(x_i, z_k, t_n)$ and $i = 1, 2, \dots, M_x - 1, k = 1, 2, \dots, M_z - 1, n = 0, 1, \dots, N - 1$.

Multiplying $[I - \frac{\tau}{2}(K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2})]$ both the right hand and left hand sides of (3.5), subtract (3.4) from the above gained formula, then we eliminate the intermediate variables $P_{i,j,k}^{n+2/3}$ and obtain an intermediate equation. Let $i = 0$ and $i = M_x$, then the additional boundary values can be obtained as

$$\begin{cases} P_{0,j,k}^{n+1/3} = P_{0,j,k}^{n+1} - \frac{\tau}{2}(K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2} + K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3})(P_{0,j,k}^{n+1} - P_{0,j,k}^n) \\ \quad + \frac{\tau^2}{4}(K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2})(K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3})(P_{0,j,k}^{n+1} - P_{0,j,k}^n), \\ P_{M_x,j,k}^{n+1/3} = P_{M_x,j,k}^{n+1} - \frac{\tau}{2}(K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2} + K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3})(P_{M_x,j,k}^{n+1} - P_{M_x,j,k}^n) \\ \quad + \frac{\tau^2}{4}(K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2})(K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3})(P_{M_x,j,k}^{n+1} - P_{M_x,j,k}^n), \end{cases} \quad (3.7)$$

where $P_{0,j,k}^n = \Phi_1(y_j, z_k, t_n)$, $P_{M_x,j,k}^n = \Phi_2(y_j, z_k, t_n)$ and $j = 1, 2, \dots, M_y - 1, k = 1, 2, \dots, M_z - 1, n = 0, 1, \dots, N - 1$.

From the three systems it can be seen that at each time step, it is just required to solve, for each fixed (j, k) (every layer in the x -direction) or each fixed (i, k) (every layer in the y -direction) or each fixed (i, j) (every layer in the z -direction), the solution of a linear system of equations with a super-triangular coefficient matrix, with $M_x - 1$ or $M_y - 1$ or $M_z - 1$ unknowns. Note that although this method can minimize the calculation, the memory is not minimized. In fact, the data of all the intermediate layers, i.e. the $(n + 1/3)$ th and $(n + 2/3)$ th layers, are used while calculating the right-hand sides of the systems (3.4) and (3.5).

3.2 Analysis of stability and consistency of the MDS

In this section, we demonstrate that the MDS (3.3–3.5) for the CSF-NUM (3.1) is an unconditionally stable scheme that has more than first-order accuracy.

The numerical solution is governed by the difference equations (3.3), (3.4) and (3.5). By eliminating the intermediate variables $P_{i,j,k}^{n+1/3}$, $P_{i,j,k}^{n+2/3}$, we obtain an equation on the whole step:

$$\left[I - \frac{\tau}{2}(K'_x \tilde{\delta}_x^{\alpha_1} + K_x \delta_x^{1+\alpha_1}) \right] \left[I - \frac{\tau}{2}(K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2}) \right] \left[I - \frac{\tau}{2}(K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3}) \right] P^{n+1}$$

$$\begin{aligned}
&= \left[I + \frac{\tau}{2} (K'_x \tilde{\delta}_x^{\alpha_1} + K_x \delta_x^{1+\alpha_1}) \right] \left[I + \frac{\tau}{2} (K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2}) \right] \left[I + \frac{\tau}{2} (K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3}) \right] P_{i,j,k}^n \\
&\quad + \frac{\tau}{2} (f_{i,j,k}^{n+1} + f_{i,j,k}^n),
\end{aligned} \tag{3.8}$$

which can be rewritten as

$$S_x S_y S_z U^{n+1} = T_x T_y T_z P^n + R^{n+1/2}, \tag{3.9}$$

where

$$\begin{aligned}
P^n = & [P_{1,1,1}^n, P_{2,1,1}^n, \dots, P_{M_x-1,1,1}^n, P_{1,2,1}^n, P_{2,2,1}^n, \dots, P_{M_x-1,2,1}^n, \dots, P_{1,M_y-1,1}^n, \\
& P_{2,M_y-1,1}^n, \dots, P_{M_x-1,M_y-1,1}^n, \\
& P_{1,1,2}^n, P_{2,1,2}^n, \dots, P_{M_x-1,1,2}^n, P_{1,2,2}^n, P_{2,2,2}^n, \dots, P_{M_x-1,2,2}^n, \dots, P_{1,M_y-1,2}^n, \\
& P_{2,M_y-1,2}^n, \dots, P_{M_x-1,M_y-1,2}^n, \\
& \dots \\
& P_{1,1,M_z-1}^n, P_{2,1,M_z-1}^n, \dots, P_{M_x-1,1,M_z-1}^n, P_{1,2,M_z-1}^n, P_{2,2,M_z-1}^n, \dots, \\
& P_{M_x-1,2,M_z-1}^n, \dots, P_{1,M_y-1,M_z-1}^n, P_{2,M_y-1,M_z-1}^n, \dots, P_{M_x-1,M_y-1,M_z-1}^n]^\top,
\end{aligned}$$

the matrices S_x, S_y, S_z and T_x, T_y, T_z represent the operators

$$I - \frac{\tau}{2} (K'_x \tilde{\delta}_x^{\alpha_1} + K_x \delta_x^{1+\alpha_1}), \quad I - \frac{\tau}{2} (K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2}), \quad I - \frac{\tau}{2} (K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3})$$

and

$$I + \frac{\tau}{2} (K'_x \tilde{\delta}_x^{\alpha_1} + K_x \delta_x^{1+\alpha_1}), \quad I + \frac{\tau}{2} (K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2}), \quad I + \frac{\tau}{2} (K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3}),$$

respectively, and the vector $R^{n+1/2}$ denotes $\frac{\tau}{2} (f^{n+1} + f^n)$.

We can consider the matrix S_x as an $(M_z - 1) \times (M_z - 1)$ block diagonal matrix, of which the blocks can be sequentially considered as $(M_y - 1) \times (M_y - 1)$ block diagonal matrix, whose blocks are the square $(M_x - 1) \times (M_x - 1)$ upper triangular matrices. We denote the j th sub-block in the k th block of S_x as $S_{j,k}^x = [(S_{j,k}^x)_{s,t}]$ for $j = 1, 2, \dots, M_y - 1, k = 1, 2, \dots, M_z - 1$.

The upper triangular matrix block $S_{j,k}^x$ entries along the s th row result from the difference equations (3.3) at the grid point (y_j, z_k) . For example, for $i = 1$ the left-hand side of the equation becomes

$$\begin{aligned}
&(-\widetilde{K}'_{x1,j,k} g_{\alpha_1,1} - \widetilde{K}_{x1,j,k} g_{1+\alpha_1,2}) P_{0,j,k}^{n+1/3} \\
&\quad + (1 - \widetilde{K}'_{x1,j,k} g_{\alpha_1,0} - \widetilde{K}_{x1,j,k} g_{1+\alpha_1,1}) P_{1,j,k}^{n+1/3} - \widetilde{K}_{x1,j,k} g_{1+\alpha_1,0} P_{2,j,k}^{n+1/3};
\end{aligned}$$

for $i = 2$, it becomes

$$\begin{aligned}
&(-\widetilde{K}'_{x2,j,k} g_{\alpha_1,2} - \widetilde{K}_{x2,j,k} g_{1+\alpha_1,3}) P_{0,j,k}^{n+1/3} + (-\widetilde{K}'_{x2,j,k} g_{\alpha_1,1} - \widetilde{K}_{x2,j,k} g_{1+\alpha_1,2}) P_{1,j,k}^{n+1/3} \\
&\quad + (1 - \widetilde{K}'_{x2,j,k} g_{\alpha_1,0} - \widetilde{K}_{x2,j,k} g_{1+\alpha_1,1}) P_{2,j,k}^{n+1/3} - \widetilde{K}_{x2,j,k} g_{1+\alpha_1,0} P_{3,j,k}^{n+1/3},
\end{aligned}$$

and for $i = M_x - 1$, we have

$$\begin{aligned} & (-\widetilde{K}'_{xM_x-1,j,k}g_{\alpha_1,M_x-1} - \widetilde{K}_{xM_x-1,j,k}g_{1+\alpha_1,M_x})P_{0,j,k}^{n+1/3} \\ & + (-\widetilde{K}'_{xM_x-1,j,k}g_{\alpha_1,M_x-2} - \widetilde{K}_{xM_x-1,j,k}g_{1+\alpha_1,M_x-1})P_{1,j,k}^{n+1/3} \\ & + \cdots + (-\widetilde{K}'_{xM_x-1,j,k}g_{\alpha_1,1} - \widetilde{K}_{xM_x-1,j,k}g_{1+\alpha_1,2})P_{M_x-2,j,k}^{n+1/3} \\ & + (1 - \widetilde{K}'_{xM_x-1,j,k}g_{\alpha_1,0} - \widetilde{K}_{xM_x-1,j,k}g_{1+\alpha_1,1})P_{M_x-1,j,k}^{n+1/3} \\ & - \widetilde{K}_{xM_x-1,j,k}g_{1+\alpha_1,0}P_{M_x,j,k}^{n+1/3}, \end{aligned}$$

where the coefficients $\widetilde{K}'_{xi,j,k} = \frac{\tau K'_{xi,j,k}}{2h_x^{\alpha_1}}$ and $\widetilde{K}_{xi,j,k} = \frac{\tau K_{xi,j,k}}{2h_x^{1+\alpha_1}}$.

Therefore, the matrix entries $S_{j,k}^x = [(S_{j,k}^x)_{s,t}]$ are given by

$$(S_{j,k}^x)_{s,t} = \begin{cases} 0, & t \geq s+2, s=1,2,\dots,M_x-3, \\ -\widetilde{K}_{xs,j,k}g_{1+\alpha_1,0}, & t=s+1, s=1,2,\dots,M_x-2, \\ 1 - \widetilde{K}'_{xs,j,k}g_{\alpha_1,0} - \widetilde{K}_{xs,j,k}g_{1+\alpha_1,1}, & t=s=1,2,\dots,M_x-1, \\ -\widetilde{K}'_{xs,j,k}g_{\alpha_1,s-t} - \widetilde{K}_{xs,j,k}g_{1+\alpha_1,s-t+1}, & t \leq s-1, s=2,3,\dots,M_x-1. \end{cases} \quad (3.10)$$

Partitioning the blocks and sub-blocks of the matrix T_x in the same way as was done for the matrix S_x , we obtain the $T_{jk}^x = [(T_{jk}^x)_{s,t}]$:

$$(T_{jk}^x)_{s,t} = \begin{cases} 0, & t \geq s+2, s=1,2,\dots,M_x-3, \\ \widetilde{K}_{xs,j,k}g_{1+\alpha_1,0}, & t=s+1, s=1,2,\dots,M_x-2, \\ 1 + \widetilde{K}'_{xs,j,k}g_{\alpha_1,0} + \widetilde{K}_{xs,j,k}g_{1+\alpha_1,1}, & t=s=1,2,\dots,M_x-1, \\ \widetilde{K}'_{xs,j,k}g_{\alpha_1,s-t} + \widetilde{K}_{xs,j,k}g_{1+\alpha_1,s-t+1}, & t \leq s-1, s=2,3,\dots,M_x-1. \end{cases} \quad (3.11)$$

Similarly, we can consider the matrix S_y as an $(M_z-1) \times (M_z-1)$ block diagonal matrix, of which the k th block, denoted as S_k^y , can be sequentially considered as an $(M_y-1) \times (M_y-1)$ block upper triangular matrix, i.e. for $t \geq s+2$, the sub-block $(S_k^y)_{s,t}$ is zero matrix and for $t \leq s+1$, the sub-block $(S_k^y)_{s,t}$ is the square $(M_x-1) \times (M_x-1)$ diagonal matrix, i.e. $(S_k^y)_{s,t} = \text{diag}((S_{1,k}^y)_{s,t}, (S_{2,k}^y)_{s,t}, \dots, (S_{M_x-1,k}^y)_{s,t})$. The same description is used for the matrix T_y . The matrix entries $S_{i,k}^y = [(S_{i,k}^y)_{s,t}]$ and $T_{i,k}^y = [(T_{i,k}^y)_{s,t}]$ can be obtained, whose form is similar to the matrices $S_{j,k}^x$ (3.10) and T_{jk}^x (3.11), respectively.

Similarly, we consider the matrix S_z as an $(M_z-1) \times (M_z-1)$ block upper triangular matrix denoted as $S_z = [(S_z)_{s,t}]$, i.e. for $t \geq s+2$, the block $(S_z)_{s,t}$ is the zero matrix and for $t \leq s+1$, the block $(S_z)_{s,t}$ is considered as an $(M_y-1) \times (M_y-1)$ block diagonal matrix whose sub-blocks are also $(M_x-1) \times (M_x-1)$ block diagonal matrices. We denote the i th element of the j th sub-block in $(S_z)_{s,t}$ as $(S_{i,j}^z)_{s,t}$.

The same way is used to propose the matrix T_z , and the matrix entries $S_{i,j}^z = [(S_{i,j}^z)_{s,t}]$ and $T_{i,j}^z = [(T_{i,j}^z)_{s,t}]$ are similar to the matrices $S_{j,k}^x$ (3.10) and T_{jk}^x (3.11), respectively.

Next we show that, if the matrices $S_x, S_y, S_z, T_x, T_y, T_z$ in (3.9) commute, i.e. the operators $I \pm \frac{\tau}{2}(K'_x \tilde{\delta}_x^{\alpha_1} + K_x \delta_x^{1+\alpha_1})$, $I \pm \frac{\tau}{2}(K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2})$, $I \pm \frac{\tau}{2}(K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3})$ commute, the MDS is unconditionally stable. The requirement for the commutativity of these operators is also a common assumption in establishing stability/convergence of a similar method for the classical higher-dimensional diffusion equation (i.e. $\alpha_1 = \alpha_2 = \alpha_3 = 2$). For example, if the diffusion coefficients are of the form with single variable $K_x = K_x(x)$, $K_y = K_y(y)$, $K_z = K_z(z)$, then these operators(matrices) commute (see Meerschaert *et al.*, 2006).

THEOREM 3.1 The MDS (3.9) for (3.1) is unconditionally stable for $0 < \alpha_1, \alpha_2, \alpha_3 < 1$ if the matrices $S_x, S_y, S_z, T_x, T_y, T_z$ commute respectively.

Proof. Rewrite the matrices S_x, S_y, S_z and T_x, T_y, T_z as

$$S_x = I - R_x, \quad T_x = I + R_x, \quad S_y = I - R_y, \quad T_y = I + R_y, \quad S_z = I - R_z, \quad T_z = I + R_z,$$

where the matrices R_x, R_y, R_z represent the operators

$$\frac{\tau}{2}(K'_x \tilde{\delta}_x^{\alpha_1} + K_x \delta_x^{1+\alpha_1}), \quad \frac{\tau}{2}(K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2}), \quad \frac{\tau}{2}(K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3}),$$

respectively.

Note that from the properties (1.10) and (1.11) of $g_{\alpha,i}$, it yields that for $0 < \alpha_1 < 1$,

$$g_{\alpha_1,0} > 0$$

and for $i \geq 1$,

$$g_{\alpha_1,i} < 0.$$

It then follows that

$$g_{\alpha_1,0} > - \sum_{i=1}^l g_{\alpha_1,i}$$

for any $l \geq 1$. From the same properties, we obtain that

$$g_{1+\alpha_1,1} < 0$$

and for $i \neq 1$,

$$g_{1+\alpha_1,i} > 0.$$

Therefore,

$$-g_{1+\alpha_1,1} > \sum_{i=0, i \neq 1}^l g_{1+\alpha_1,i}$$

for any $l > 1$. Considering the blocks and sub-blocks of R_x similar to those of S_x in the above, the eigenvalues of R_x are in the discs centred at

$$(R_{j,k}^x)_{s,s} = \widetilde{K}_{xs,j,k}' g_{\alpha_1,0} + \widetilde{K}_{xs,j,k} g_{1+\alpha_1,1},$$

with radius

$$\begin{aligned} r_s &= \sum_{l=1, l \neq s}^{M_x-1} |(R_{j,k}^x)_{s,l}| \leq - \sum_{l=1, l \neq s}^s \widetilde{K}'_{xs,j,k} g_{a_1,s-l} - \sum_{l=1, l \neq s}^{s+1} \widetilde{K}_{xs,j,k} g_{1+a_1,s-l+1} \\ &< -\widetilde{K}'_{xs,j,k} g_{a_1,0} - \widetilde{K}_{xs,j,k} g_{1+a_1,1} \end{aligned}$$

since $\widetilde{K}'_{xs,j,k} \leq 0$, $\widetilde{K}_{xs,j,k} > 0$, $s = 1, 2, \dots, M_x - 1$, $j = 1, 2, \dots, M_y - 1$, $k = 1, 2, \dots, M_z - 1$. From the Gerschgorin theorem (see [Demmel, 1997](#)), each eigenvalue of the matrix R_x has a negative real part.

Note that ρ is an eigenvalue of R_x if and only if $(1 - \rho)$ is an eigenvalue of the matrix $S_x = I - R_x$ and if and only if $\frac{1+\rho}{1-\rho}$ is an eigenvalue of the matrix $S_x^{-1}T_x = (I - R_x)^{-1}(I + R_x)$. Then the eigenvalue of the matrix $S_x^{-1}T_x$ has a modulus less than 1. Therefore, the spectral radius of the matrix $S_x^{-1}T_x$ is less than 1.

Similarly, we can also obtain that the spectral radii of the matrices $S_y^{-1}T_y$ and $S_z^{-1}T_z$ are less than 1.

We assume that the initial error ε^0 is introduced only when the initial condition is discretized. Thus, the error ε^n , which is accumulated from the initial error ε^0 in the course of solving the solution in (3.9), satisfies

$$S_x S_y S_z \varepsilon^n = T_x T_y T_z \varepsilon^{n-1}$$

or

$$\varepsilon^n = (S_x^{-1} S_y^{-1} S_z^{-1} T_x T_y T_z)^n \varepsilon^0.$$

When the matrices S_x, S_y, S_z and T_x, T_y, T_z commute, i.e. $S_x^{-1}, S_y^{-1}, S_z^{-1}$ and T_x, T_y, T_z commute, we have

$$\varepsilon^n = (S_x^{-1} T_x)^n (S_y^{-1} T_y)^n (S_z^{-1} T_z)^n \varepsilon^0.$$

As the spectral radii of the matrices $S_x^{-1} T_x, S_y^{-1} T_y, S_z^{-1} T_z$ are less than 1, it follows that

$$(S_x^{-1} T_x)^n \rightarrow \mathbf{0}, \quad (S_y^{-1} T_y)^n \rightarrow \mathbf{0}, \quad (S_z^{-1} T_z)^n \rightarrow \mathbf{0} \quad \text{as } n \rightarrow \infty,$$

where $\mathbf{0}$ denotes the zero matrix. Therefore, the stability of the MDS follows. □

Taking the consistency of the MDS (3.8) into account, we write its equivalent form:

$$\begin{aligned} \frac{P_{i,j,k}^{n+1} - P_{i,j,k}^n}{\tau} &= (K'_x \widetilde{\delta}_x^{a_1} + K_x \delta_x^{1+a_1} + K'_y \widetilde{\delta}_y^{a_2} + K_y \delta_y^{1+a_2} + K'_z \widetilde{\delta}_z^{a_3} + K_z \delta_z^{1+a_3}) \frac{P_{i,j,k}^{n+1} + P_{i,j,k}^n}{2} \\ &\quad - \frac{\tau^2}{4} [(K'_x \widetilde{\delta}_x^{a_1} + K_x \delta_x^{1+a_1})(K'_y \widetilde{\delta}_y^{a_2} + K_y \delta_y^{1+a_2}) + (K'_x \widetilde{\delta}_x^{a_1} + K_x \delta_x^{1+a_1})(K'_z \widetilde{\delta}_z^{a_3} + K_z \delta_z^{1+a_3}) \\ &\quad + (K'_y \widetilde{\delta}_y^{a_2} + K_y \delta_y^{1+a_2})(K'_z \widetilde{\delta}_z^{a_3} + K_z \delta_z^{1+a_3})] \frac{P_{i,j,k}^{n+1} - P_{i,j,k}^n}{\tau} + \frac{\tau^3}{8} (K'_x \widetilde{\delta}_x^{a_1} + K_x \delta_x^{1+a_1}) \\ &\quad \times (K'_y \widetilde{\delta}_y^{a_2} + K_y \delta_y^{1+a_2})(K'_z \widetilde{\delta}_z^{a_3} + K_z \delta_z^{1+a_3})(P_{i,j,k}^{n+1} + P_{i,j,k}^n) + \frac{\tau}{2} (f_{i,j,k}^{n+1} + f_{i,j,k}^n). \end{aligned} \quad (3.12)$$

Note that the above form is a Crank–Nicolson scheme added with a modified perturbed term with approximation order $O(\tau^2)$, so the time difference operator has a local truncation error with $O(\tau^2)$, which is obtained from the Taylor expansion when the first-order time derivative is approximated by the central difference. The six spatial differential operators (3.2) have local truncation error with $O(h_x)$, $O(h_y)$ and $O(h_z)$, respectively, which were proved in Meerschaert & Tadjeran (2004).

Above we have shown that the MDS is consistent and stable, then by Lax's equivalence theorem (see Smith, 1990), it converges at the rate $O(\tau^2) + O(h_x) + O(h_y) + O(h_z)$.

3.3 Improving the speed of convergence by Richardson extrapolation

In this section, we improve the speed of convergence using Richardson extrapolation, we find it to be worthwhile to recall here the following useful lemma associated with error estimate referred to in Tadjeran *et al.* (2006).

LEMMA 3.2 Let $1 < \alpha < 2$ and $f \in C^{n+3}(R)$ such that all derivatives of f up to order $n + 3$ belong to $L^1(R)$. For any integer $p \geq 0$, we define the shifted Grünwald difference operator by

$$\Delta_{h,p}^\alpha f(x) = \sum_{j=0}^{\infty} g_{\alpha,j} f(x - (j - p)h).$$

Then if the left side of the domain is $-\infty$, we have for some constants a_l independent of h, f, x that

$$h^{-\alpha} \Delta_{h,p}^\alpha f(x) = \frac{d^\alpha}{dx^\alpha} f(x) + \sum_{l=1}^{n-1} \left(a_l \frac{d^{\alpha+l}}{dx^{\alpha+l}} f(x) \right) h^l + O(h^n)$$

uniformly in $x \in R$.

We can establish the same proposition under the case $0 < \alpha < 1$. And then from Lemma 3.2 and (3.12), we obtain the truncation error of the MDS (3.9):

$$\begin{aligned} & -\frac{P_{i,j,k}^{n+1} - P_{i,j,k}^n}{\tau} + (K'_x \tilde{\delta}_x^{\alpha_1} + K_x \delta_x^{1+\alpha_1} + K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2} + K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3}) \frac{P_{i,j,k}^{n+1} + P_{i,j,k}^n}{2} + O(\tau^2) \\ &= -\left[\frac{\partial P}{\partial t} \right]_{i,j,k}^n + K'_x \left[\frac{\partial^{\alpha_1} P}{\partial x^{\alpha_1}} \right]_{i,j,k}^{n+1/2} + K'_x a_1 \left[\frac{\partial^{1+\alpha_1} P}{\partial x^{1+\alpha_1}} \right]_{i,j,k}^{n+1/2} h_x + K'_x a_2 \left[\frac{\partial^{2+\alpha_1} P}{\partial x^{2+\alpha_1}} \right]_{i,j,k}^{n+1/2} h_x^2 \\ &+ K_x \left[\frac{\partial^{1+\alpha_1} P}{\partial x^{1+\alpha_1}} \right]_{i,j,k}^{n+1/2} + K_x b_1 \left[\frac{\partial^{2+\alpha_1} P}{\partial x^{2+\alpha_1}} \right]_{i,j,k}^{n+1/2} h_x + K_x b_2 \left[\frac{\partial^{3+\alpha_1} P}{\partial x^{3+\alpha_1}} \right]_{i,j,k}^{n+1/2} h_x^2 \\ &+ K'_y \left[\frac{\partial^{\alpha_2} P}{\partial y^{\alpha_2}} \right]_{i,j,k}^{n+1/2} + K'_y c_1 \left[\frac{\partial^{1+\alpha_2} P}{\partial y^{1+\alpha_2}} \right]_{i,j,k}^{n+1/2} h_y + K'_y c_2 \left[\frac{\partial^{2+\alpha_2} P}{\partial y^{2+\alpha_2}} \right]_{i,j,k}^{n+1/2} h_y^2 \\ &+ K_y \left[\frac{\partial^{1+\alpha_2} P}{\partial y^{1+\alpha_2}} \right]_{i,j,k}^{n+1/2} + K_y d_1 \left[\frac{\partial^{2+\alpha_2} P}{\partial y^{2+\alpha_2}} \right]_{i,j,k}^{n+1/2} h_y + K_y d_2 \left[\frac{\partial^{3+\alpha_2} P}{\partial x^{3+\alpha_2}} \right]_{i,j,k}^{n+1/2} h_y^2 \end{aligned}$$

$$\begin{aligned}
& + K'_z \left[\frac{\partial^{\alpha_3} P}{\partial z^{\alpha_3}} \right]_{i,j,k}^{n+1/2} + K'_z e_1 \left[\frac{\partial^{1+\alpha_3} P}{\partial z^{1+\alpha_3}} \right]_{i,j,k}^{n+1/2} h_z + K'_z e_2 \left[\frac{\partial^{2+\alpha_3} P}{\partial z^{2+\alpha_3}} \right]_{i,j,k}^{n+1/2} h_z^2 \\
& + K_z \left[\frac{\partial^{1+\alpha_3} P}{\partial z^{1+\alpha_3}} \right]_{i,j,k}^{n+1/2} + K_z f_1 \left[\frac{\partial^{2+\alpha_3} P}{\partial z^{2+\alpha_3}} \right]_{i,j,k}^{n+1/2} h_z + K_z f_2 \left[\frac{\partial^{3+\alpha_3} P}{\partial z^{3+\alpha_3}} \right]_{i,j,k}^{n+1/2} h_z^2 \\
& + O(\tau^2) + O(h_x^3) + O(h_y^3) + O(h_z^3),
\end{aligned}$$

i.e.

$$\begin{aligned}
& - \frac{P_{i,j,k}^{n+1} - P_{i,j,k}^n}{\tau} + (K'_x \tilde{\delta}_x^{\alpha_1} + K_x \delta_x^{1+\alpha_1} + K'_y \tilde{\delta}_y^{\alpha_2} + K_y \delta_y^{1+\alpha_2} + K'_z \tilde{\delta}_z^{\alpha_3} + K_z \delta_z^{1+\alpha_3}) \frac{P_{i,j,k}^{n+1} + P_{i,j,k}^n}{2} \\
& = - \left[\frac{\partial P}{\partial t} \right]_{i,j,k}^n + K'_x \left[\frac{\partial^{\alpha_1} P}{\partial x^{\alpha_1}} \right]_{i,j,k}^{n+1/2} + K_x \left[\frac{\partial^{1+\alpha_1} P}{\partial x^{1+\alpha_1}} \right]_{i,j,k}^{n+1/2} + K'_y \left[\frac{\partial^{\alpha_2} P}{\partial y^{\alpha_2}} \right]_{i,j,k}^{n+1/2} \\
& + K_y \left[\frac{\partial^{1+\alpha_2} P}{\partial y^{1+\alpha_2}} \right]_{i,j,k}^{n+1/2} + K'_z \left[\frac{\partial^{\alpha_3} P}{\partial z^{\alpha_3}} \right]_{i,j,k}^{n+1/2} + K_z \left[\frac{\partial^{1+\alpha_3} P}{\partial z^{1+\alpha_3}} \right]_{i,j,k}^{n+1/2} \\
& + (a'_1 + b'_1)h_x + (a'_2 + b'_2)h_x^2 + (c'_1 + d'_1)h_y + (c'_2 + d'_2)h_y^2 + (e'_1 + f'_1)h_z + (e'_2 + f'_2)h_z^2 \\
& + O(\tau^2) + O(h_x^3) + O(h_y^3) + O(h_z^3),
\end{aligned}$$

where $\left[\frac{\partial^\gamma P}{\partial x^\gamma} \right]^{n+1/2}$ denotes $(\left[\frac{\partial^\gamma P}{\partial x^\gamma} \right]^{n+1} + \left[\frac{\partial^\gamma P}{\partial x^\gamma} \right]^n)/2$ and the constants $a'_1, a'_2, b'_1, b'_2, c'_1, c'_2, d'_1, d'_2, e'_1, e'_2, f'_1, f'_2$ do not depend on the spatial steps h_x, h_y, h_z .

By the Lax theorem (see [Thomas, 1995](#)), we obtain the relation between the numerical solution P_h and the exact solution $P(x, y, z, t)$:

$$\begin{aligned}
P_h & = P(x, y, z, t) + (a'_1 + b'_1)h_x + (a'_2 + b'_2)h_x^2 + (c'_1 + d'_1)h_y \\
& + (c'_2 + d'_2)h_y^2 + (e'_1 + f'_1)h_z + (e'_2 + f'_2)h_z^2 + O(\tau^2) \\
& + O(h_x^3) + O(h_y^3) + O(h_z^3).
\end{aligned} \tag{3.13}$$

Applying the MDS with half spatial steps $h_x/2, h_y/2, h_z/2$, we suppose that the corresponding numerical solution is denoted by $P_{h/2}$:

$$\begin{aligned}
P_{h/2} & = P(x, y, z, t) + (a'_1 + b'_1)\frac{h_x}{2} + (a'_2 + b'_2)\frac{h_x^2}{4} + (c'_1 + d'_1)\frac{h_y}{2} \\
& + (c'_2 + d'_2)\frac{h_y^2}{4} + (e'_1 + f'_1)\frac{h_z}{2} + (e'_2 + f'_2)\frac{h_z^2}{4} \\
& + O(\tau^2) + O(h_x^3) + O(h_y^3) + O(h_z^3).
\end{aligned} \tag{3.14}$$

Subtracting (3.13) from twice (3.14), the extrapolated solution is then computed from $\tilde{P} = 2P_{h/2} - P_h$ and the truncation error is $O(\tau^2) + O(h_x^2) + O(h_y^2) + O(h_z^2)$.

4. Numerical examples

In this section, some numerical results are presented to support our theoretical analysis.

EXAMPLE 4.1 The following NCSF-UM is considered:

$$\frac{\partial P(x, y, z, t)}{\partial t} = K_x \frac{\partial^{1.8} P(x, y, z, t)}{\partial x^{1.8}} + K_y \frac{\partial^{1.8} P(x, y, z, t)}{\partial y^{1.8}} + K_z \frac{\partial^{1.8} P(x, y, z, t)}{\partial z^{1.8}} + c_0 \delta_0(x_0, y_0, z, t_0)$$

$$(0 \leq x \leq 1000, 0 \leq y \leq 1000, 0 \leq z \leq 1000, 0 < t < T), \quad (4.1)$$

with the initial and boundary conditions

$$P(x, y, z, 0) = P(x, y, z, t)|_{\Gamma} = 0, \quad (4.2)$$

where $c_0 = 40$ and $x_0 = y_0 = t_0 = 0$.

The FADIS is used to solve (4.1). The numerical simulation of the diffusion process is shown in Figs 1–3, respectively. As the time t increases, one observes that the source diffuses.

By contrast to Fig. 3, Fig. 4 shows a different diffusion process with different seepage flow coefficients. When the coefficients are smaller, the diffusion process is much slower (Fig. 4).

In Fig. 5, we exhibit the difference between the seepage flow in anisotropic and isotropic porous media. The seepage flow diffusion speed in isotropic porous media is uniform in both the x -direction and the y -direction (Fig. 4). However, for the anisotropic porous medium, the speed in the x -direction is not the same as the y -direction (Fig. 5).

In order to show the approximation order of the FADIS, we construct an example with an analytic solution.

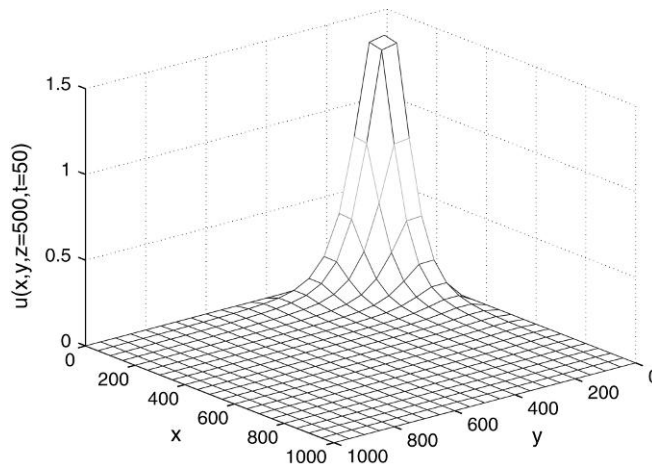
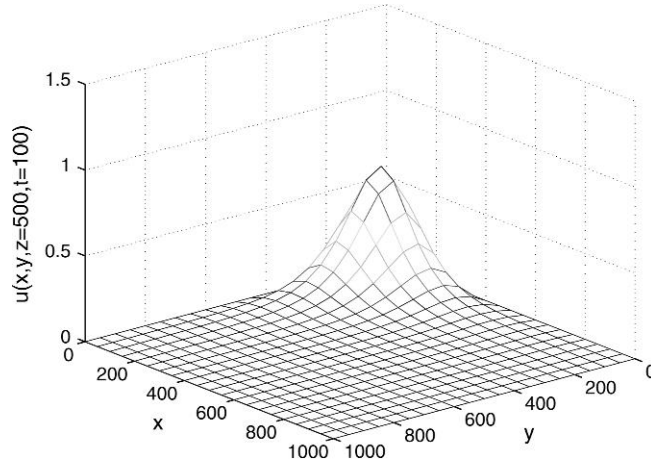
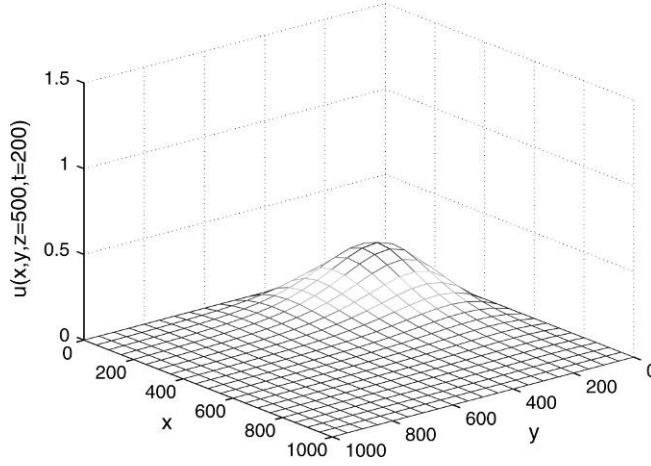


FIG. 1. Numerical solution for $K_x = K_y = K_z = 40$, $t = 50$ at $z = 500$.

FIG. 2. Numerical solution for $K_x = K_y = K_z = 40$, $t = 100$ at $z = 500$.FIG. 3. Numerical solution for $K_x = K_y = K_z = 40$, $t = 200$ at $z = 500$.

EXAMPLE 4.2 The following non-continued seepage flow with analytic solution in uniform media is considered:

$$\frac{\partial P(x, y, z, t)}{\partial t} = K_x \frac{\partial^{1.8} P(x, y, z, t)}{\partial x^{1.8}} + K_y \frac{\partial^{1.8} P(x, y, z, t)}{\partial y^{1.8}} + K_z \frac{\partial^{1.6} P(x, y, z, t)}{\partial z^{1.6}} + f(x, y, z, t)$$

$$(0 \leq x \leq 1, 0 \leq y \leq 1, 0 \leq z \leq 1, t > 0),$$

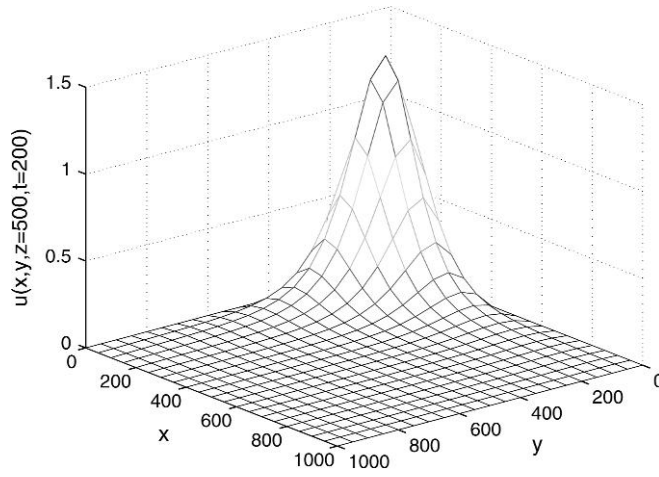


FIG. 4. Numerical solution for $K_x = K_y = K_z = 20$, $t = 200$ at $z = 500$.

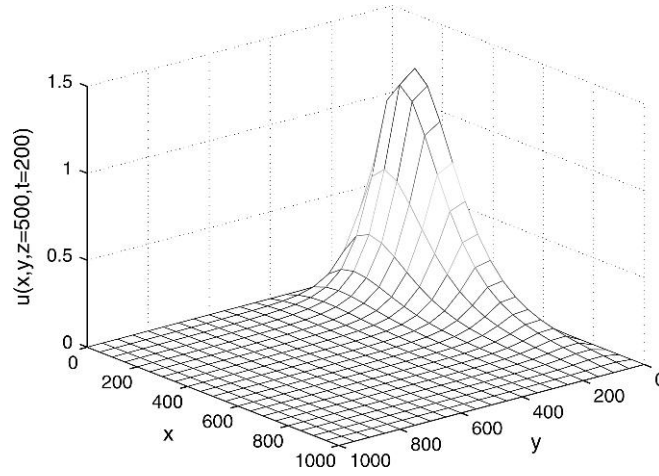


FIG. 5. Numerical solution for $K_x = 10$, $K_y = K_z = 40$, $t = 200$ at $z = 500$.

where

$$K_x = 0.1\Gamma(1.4)/\Gamma(3.2),$$

$$K_y = 0.1\Gamma(1.2)/\Gamma(3),$$

$$K_z = 0.1\Gamma(1.4)/\Gamma(3),$$

$$f(x, y, t) = -e^{-t}x^{2.2}y^2z^2 - 0.1e^{-t}x^{0.4}y^2z^2 - 0.1e^{-t}x^2y^{0.2}z^2 - 0.1e^{-t}x^2y^2z^{0.4},$$

with the initial and boundary conditions

$$\begin{aligned}
 P(x, y, z, 0) &= x^{2.2} y^{2.0} z^{2.0}, \\
 P(0, y, z, t) &= P(x, 0, z, t) = P(x, y, 0, t) = 0, \\
 P(1, y, z, t) &= e^{-t} y^{2.0} z^{2.0}, \\
 P(x, 1, z, t) &= e^{-t} x^{2.2} z^{2.0}, \\
 P(x, y, 1, t) &= e^{-t} x^{2.2} y^{2.0}.
 \end{aligned}$$

The analytic solution of this problem is

$$P(x, y, z, t) = e^{-t} x^{2.2} y^{2.0} z^{2.0}.$$

The maximum absolute error between the exact solution and the numerical solutions by FADIS, with spatial and temporal steps $\tau = h_x = h_y = h_z = 1/10, 1/20, 1/40$ at time $t = 1.0$, is listed in Table 1.

Table 1 shows the numerical errors at $t = 1$ between the exact solution and the numerical solution FADIS. From Table 1, it can be seen that

$$\text{Error rate} = \frac{\text{error}_1}{\text{error}_2} \approx \frac{h_1}{h_2} = 2.$$

Thus, we obtain that the order of convergence of the numerical method FADIS is $(\log_2 2 = 1)$ first order, i.e. the convergence order of the numerical method FADIS is $O(\tau + h_x + h_y + h_z)$.

This is in good agreement with our theoretical analysis.

EXAMPLE 4.3 The following CSF-NUM is considered:

$$\begin{aligned}
 \frac{\partial P(x, y, z, t)}{\partial t} &= \frac{\partial}{\partial x} \left(K_x(x, y, z) \frac{\partial^{0.8} P(x, y, z, t)}{\partial x^{0.8}} \right) + \frac{\partial}{\partial y} \left(K_y(x, y, z) \frac{\partial^{0.8} P(x, y, z, t)}{\partial y^{0.8}} \right) \\
 &\quad + \frac{\partial}{\partial z} \left(K_z(x, y, z) \frac{\partial^{0.6} P(x, y, z, t)}{\partial z^{0.6}} \right) + f(x, y, z, t) \\
 (0 \leq x \leq 1, 0 \leq y \leq 1, 0 \leq z \leq 1, t > 0),
 \end{aligned} \tag{4.3}$$

TABLE 1 Comparison of maximum error for FADIS at time $t = 1.0$

$\tau = h_x = h_y = h_z$	Maximum error	Error rate
$\frac{1}{10}$	0.00323693	—
$\frac{1}{20}$	0.00191495	$1.7 \approx 2$
$\frac{1}{40}$	0.00010339	$1.9 \approx 2$

where

$$\begin{aligned} K_x(x, y, z) &= (2 - x^2)yz, \quad K_y(x, y, z) = x(2 - y^2)z, \quad K_z(x, y, z) = xy(2 - z^2), \\ f(x, y, z, t) &= -e^{-t}(-2\Gamma(3.2)/\Gamma(2.4)x^{2.4}y^3z^3 + \Gamma(3.2)/\Gamma(1.4)x^{0.4}y^3z^3(2 - x^2) \\ &\quad - 2\Gamma(3)/\Gamma(2.2)x^{3.2}y^{2.2}z^3 + \Gamma(3)/\Gamma(1.2)x^{3.2}y^{0.2}z^3(2 - y^2) \\ &\quad - 2\Gamma(3)/\Gamma(2.4)x^{3.2}y^3z^{2.4} + \Gamma(3)/\Gamma(1.4)x^{3.2}y^3z^{0.4}(2 - z^2)) \end{aligned}$$

with the initial and boundary conditions

$$\begin{aligned} P(x, y, z, 0) &= x^{2.2}y^{2.0}z^{2.0}, \\ P(0, y, z, t) &= P(x, 0, z, t) = P(x, y, 0, t) = 0, \\ P(1, y, z, t) &= e^{-t}y^{2.0}z^{2.0}, \\ P(x, 1, z, t) &= e^{-t}x^{2.2}z^{2.0}, \\ P(x, y, 1, t) &= e^{-t}x^{2.2}y^{2.0}. \end{aligned} \tag{4.4}$$

The analytic solution of this problem is

$$P(x, y, t) = e^{-t}x^{2.2}y^2z^2,$$

which can be verified by substituting directly into (4.3).

Table 2 shows the numerical errors at $t = 1$ between the exact solution and the numerical solutions obtained by the MDS and the MDS with a Richardson extrapolation (MDS-R-Ext). From Table 2, both the two numerical methods with $h_x = h_y = h_z = \tau = 1/4, 1/8, 1/16$ are in excellent agreement with the exact solution.

From Table 2, it can be seen that

$$\text{Error rate of MDS} = \frac{\text{error}_1}{\text{error}_2} \approx \frac{h_1}{h_2} = 2$$

and

$$\text{Error rate of MDS-R-Ext} = \frac{\text{error}_1}{\text{error}_2} \approx \left(\frac{h_1}{h_2}\right)^2 = 4.$$

Thus, we obtain that the order of convergence of the numerical method MDS is ($\log_2 2 = 1$) first order and the order of convergence of the numerical method MDS-R-Ext is ($\log_2 4 = 2$) second order,

TABLE 2 Comparison of maximum errors (MERR) and Error rate (ER) for MDS and MDS-R-Ext (MExt) at time $t = 1.0$

$\tau = h_x = h_y = h_z$	MERR-MDS	ER-MDS	MERR-MExt	ER-MExt
$\frac{1}{5}$	0.00310914	—	0.00183068	—
$\frac{1}{10}$	0.00153984	2.02	0.000438217	$4.18 \approx 4$
$\frac{1}{20}$	0.000807034	1.91	0.000108119	$4.05 \approx 4$

i.e. the order of convergence of the numerical method MDS is $O(\tau^2 + h_x + h_y + h_z)$ and the order of convergence of the numerical method MDS-R-Ext is $O(\tau^2 + h_x^2 + h_y^2 + h_z^2)$.

These results are in good agreement with our theoretical analysis.

From Example 4.3, it can be seen that the stability result can be obtained even if the commutativity of the matrices is not satisfied. Note that Example 4.3 does not meet the requirement for the commutativity of these operators which was used to establish the stability of the MDS method. The convergence of the numerical solution for this example suggests that the stability results may be extended beyond the requirement for commutativity (see also [Meerschaert et al., 2006](#)).

An additional numerical experiment is presented, which investigates specifically the phenomenon of ‘seepage’ flow. Here we show the simulation results at $t = 16$ and $z = 0.5$ for the case where the specific storage coefficient $\frac{1}{v} = 10^{-2}$ and $\frac{1}{v} = 10^{-6}$ in (4.5).

EXAMPLE 4.4 (see [He, 1998](#))

$$\frac{1}{v} \frac{\partial P(x, y, z, t)}{\partial t} = \frac{\partial}{\partial x} \left(\frac{\partial^{0.5} P(x, y, z, t)}{\partial x^{0.5}} \right) + \frac{\partial}{\partial y} \left(\frac{\partial^{0.5} P(x, y, z, t)}{\partial y^{0.5}} \right) + \frac{\partial}{\partial z} \left(\frac{\partial^{0.5} P(x, y, z, t)}{\partial z^{0.5}} \right) \\ (0 \leq x \leq 1, 0 \leq y \leq 1, 0 \leq z \leq 1, t > 0), \quad (4.5)$$

with the initial and boundary conditions

$$\begin{aligned} P(x, y, z, 0) &= 0 \\ P(0, y, z, t) &= P(x, 0, z, t) = P(x, y, 0, t) = 0, \\ P(1, y, z, t) &= y^{\frac{3}{2}} z^{\frac{3}{2}} \frac{\sqrt{3\pi t}}{4}, \\ P(x, 1, z, t) &= x^{\frac{3}{2}} z^{\frac{3}{2}} \frac{\sqrt{3\pi t}}{4}, \\ P(x, y, 1, t) &= x^{\frac{3}{2}} y^{\frac{3}{2}} \frac{\sqrt{3\pi t}}{4}. \end{aligned} \quad (4.6)$$

The MDS is used to solve (4.5–4.6). The numerical simulations of the percolation process are shown in Figs 6–8, where we take the specific storage coefficient $\frac{1}{v} = 10^{-2}$.

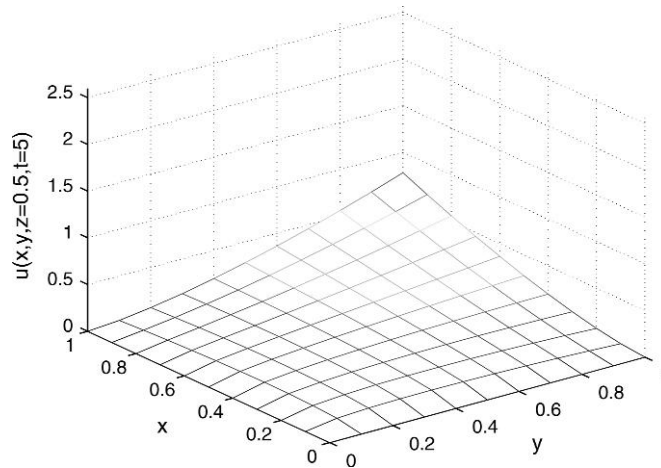


FIG. 6. Numerical solution for $\frac{1}{v} = 10^{-2}$, $t = 5$ at $z = 0.5$.

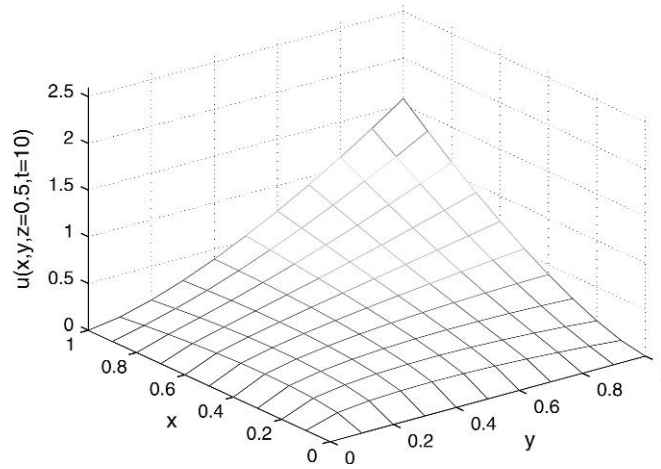


FIG. 7. Numerical solution for $\frac{1}{v} = 10^{-2}$, $t = 10$ at $z = 0.5$.

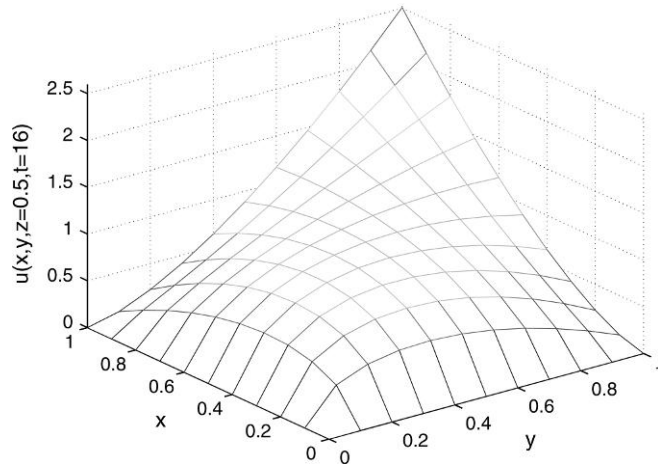


FIG. 8. Numerical solution for $\frac{1}{v} = 10^{-2}$, $t = 16$ at $z = 0.5$.

By contrast to Fig. 8, Fig. 9 shows a different percolation process with different specific storage coefficient, i.e. $\frac{1}{v} = 10^{-2}$ and $\frac{1}{v} = 10^{-6}$ at time $t = 16$.

5. Conclusions

In this paper, an FADIS for the NCSF-UM and MDS for the CSF-NUM in three dimensions have been described and demonstrated. The stability, consistency and convergence of the FADIS and MDS have been discussed. An improvement of the speed of convergence of the MDS by Richardson extrapolation is also presented. The FADIS and both the MDS and the MDS-R-Ext techniques provide computationally effective tools for simulating the behaviour of the solution of the NCSF-UM and the CSF-NUM,

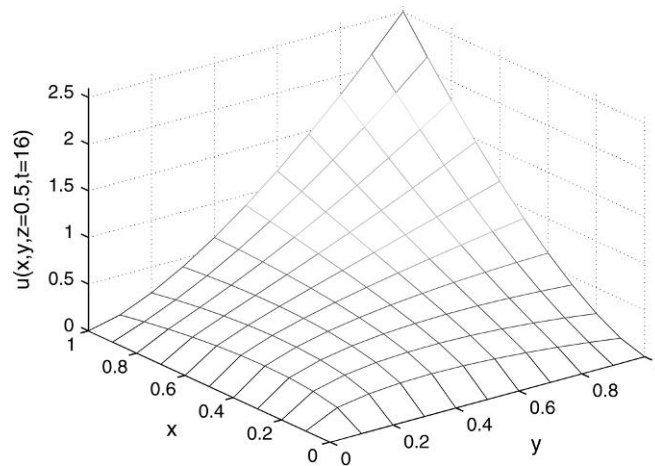


FIG. 9. Numerical solution for $\frac{1}{\nu} = 10^{-6}$, $t = 16$ at $z = 0.5$.

respectively. These methods and analytical techniques can also be extended to some high-dimensional fractional PDEs.

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